Number of isomers.

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The number of structural isomers for an alkane molecule will always be less than 2^(n-1), where n is the number of carbon atoms. The exact formula can be strictly derived; this requires the help of mathematicians specializing in combinatorics. Next, we'll look at how to accurately count isomers.

To understand, it is enough to analyze the number of isomers for the pentane molecule (n = 5).

Pentane has three structural isomers. Here are their formulas:

1. $CH_3 – CH_2 – CH_2 – CH_2 – CH_3$
2. $CH_3 – CH(CH_3) – CH_2 – CH_3$
3. $CH_3 – C(CH_3)_2 – CH_3$

Let's translate the formulas into numbers, for this we will count the number of carbon atoms. Then for the above formulas we get:

1. 1 + 1 + 1 + 1 + 1 = 5
2. 1 + 2 + 1 + 1 = 5
3. 1 + 3 + 1 = 5

In combinatorics, such a decomposition is called the composition of a number (when the order of the parts is taken into account).

"In number theory, the composition, or decomposition, of a natural number is its representation in the form of a sum of natural numbers, which takes into account the order of the terms.

The components included in the composition are called parts, and their number is the length of the composition.

Partitioning a number, unlike composition, does not take into account the order of the parts. Consequently, the number of partitions of a number never exceeds the number of compositions..." [1].

Let us now consider all compositions of the number 5. Let us list all 16 options (data from the above link).

5 =

4 + 1 =

3 + 2 =

3 + 1 + 1 =

2 + 3 =

2 + 2 + 1 =

2 + 1 + 2 =

2 + 1 + 1 + 1 =

1 + 4 =

1 + 3 + 1 =

1 + 2 + 2 =

1 + 2 + 1 + 1 =

1 + 1 + 3 =

1 + 1 + 2 + 1 =

1 + 1 + 1 + 2 =

1 + 1 + 1 + 1 + 1 =

Further, let us note that in order to calculate the number of isomers, it is necessary to take into account only those compositions that begin and end with a unit, since alkane molecules begin and end with the –CH3 group, that is, with a unit. Here are these 4 compositions.

1 + 3 + 1 =

1 + 2 + 1 + 1 =

1 + 1 + 2 + 1 =

1 + 1 + 1 + 1 + 1 =

Now let's take into account that the two compositions are equivalent, since they represent one isomer - isopentane.

CH_3 – CH (CH_3) – CH_2 – CH_3

1 + 2 + 1 + 1 = 5

1 + 1 + 2 + 1 = 5

As a result, we get three compositions that absolutely correctly represent the 3 isomers of pentane (5):

1 + 3 + 1 =

1 + 2 + 1 + 1 =

1 + 1 + 1 + 1 + 1 =

In general, it is also necessary to take into account that the length of any composition must be greater than the length of the side radicals (or equal) - this follows from the nomenclature of alkanes. Taking this condition into account will discard many “empty” composition options.

Now, I think, the algorithm for deriving the formula is absolutely clear. Moreover, it is obvious that the number of structural isomers will always be less than the number of compositions, that is, less than the number 2^(n-1), where n is the number of carbon atoms in the alkane molecule. This can be verified by comparing the number of structural isomers for a given number of carbon atoms and the number of composition options.

It is necessary to point out that in general, numbers in a composition greater than 2 may represent different isomers, since the substituents themselves are subject to isomerism. Let's explain using the example of the propyl radical, that is, when the number is 4 (3 + 1, 1 - the main chain). Here are all the combinations, if we have the number 4 (propyl radical) in the composition:

$CH_3 – CH_2 – CH_2$-

CH_3 – CH(-) – CH_3

CH_3 - , $CH_3 – CH_2$ -

That is, we have 3 options.

3

3(i)

1 + 2

Let's consider the butyl radical, that is, when the number 5 is in the composition (4 + 1, 1 is the main chain).

$CH_3 – CH_2 –CH_2 –CH_2$ –

CH_3 – CH(-) – $CH_2 – CH_3$

CH_3 – CH(CH_3) – CH_2 -

CH_3 - , $CH_3 –CH_2 –CH_2$ -

CH_3 - , CH_3 – CH(-) – CH_3

$CH_3 – CH_2$ - , $CH_3 – CH_2$ –

That is, there are 6 options when the number 5 is in the composition.

4

4(i)

1 + 2 + 1

1 + 3

1 + 3(i)

2 + 2

In fact, it is necessary to take into account the structural isomerism of the radicals themselves and the division of radicals into two parts when the composition contains numbers greater than two ($\lambda > 2$).

$n = \lambda 1 + \lambda 2 + \lambda 3 + \ldots + \lambda n$

Therefore, the derivation of the exact formula for the number of alkane isomers can be done based on the composition of the number (n), but it is necessary to take into account at what numbers the isomers are equivalent (for example, at 2), and the fact that the length of the composition is greater than the length of the radicals (or equal).

You also need to take into account the number of isomers depending on the radical (4, 5, etc.), and analyze how this relates to the number of isomers. In any case, this can be analyzed and taken into account.

But, it is quite obvious that the number of structural isomers of alkanes is a composition of the number n (n is the number of carbon atoms), although with some conditions. Therefore, the derivation of the formula must be successful.

I note that the algorithm for a computer is elementary, and therefore you can write a program that will calculate the number of structural isomers for alkane molecules.

The computer will also count the number of stereoisomers, since the counting formula is well known: 2^n, where n is the number of asymmetric carbon atoms (that is, carbon atoms with 4 different substituents).

When such formulas are obtained, all other homological series are derived and programmed similarly.

1. Composition (combinatorics). Wikipedia (ru). https://en.wikipedia.org/wiki/Composition_(combinatorics)